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Ab initio studying of topological insulator Bi2Se3 under the stress

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Abstract

A topological insulator is an unusual state of quantum matter which, while being an insulator in the bulk, has topologically protected electronic states at the surface. These states could be used in different applications, such as spintronics and quantum computing. However, it is difficult to distinguish the surface and bulk contributions into transport properties, such as conductivity. In order to distinguish surface and bulk contributions an external pressure could be applied. In the present work we have performed ab initio calculations of topological insulator Bi2Se3 under the stress for bulk and surface models. Calculations have been made by means of density functional theory within generalized gradient approximation, the spin-orbit interaction was taken into account as well. It was found that topologically protected surface states remains robust under the stress. Moreover, pressure tends to increase the Fermi velocity of surface electrons, as well as increase electronic density of states at the bottom of the conduction band of the bulk of Bi2Se 3. Thus, the results of ab initio calculations could complement the experimental investigations of high pressure transport properties of topological insulators. The experimentally detected increase of carrier density could be related to the effects of the bulk.

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